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## Quantum chemical studies of the physics around the metal-insulator transition in (EDO-TTF)2PF6

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Stellingen  
behorende bij het proefschrift  
Quantum chemical studies of the physics  
around the metal-insulator transition  
in (EDO-TTF)<sub>2</sub>PF<sub>6</sub>  
van  
Gerrit-Jan Linker  
Nieuw-Amsterdam, 7 oktober 2016

1. Water molecules do not have rabbit ears, even when there is cabbage nearby.
2. “Non-classical bond angles” [1] can be understood classically. Using our classical model for the bond angle, the extended Debye polarisability model [2], it can be understood why the cumulene C=C=C=C is linear while O=C=C=C=O has a C<sub>2v</sub> symmetry.  
1: “Nonclassical distortions at multiple bonds”, G. Trinquier, J.P. Malrieu. *J. Am. Chem. Soc.* 109 (1987), 18, 5303 ;  
2: “Off-Planar Geometry and Structural Instability of EDO-TTF Explained by Using the Extended Debye Polarizability Model for Bond Angles”, G.J. Linker, P.Th. van Duijnen, P.H.M. van Loosdrecht, R. Broer
3. We have no direct access to reality. What can be observed directly, *e.g.* in empirical experiments, are projections, or shadows. Models based on theory can provide additional projections of reality.<sup>a</sup>
4. A cluster model is a bad model for the bulk when the frontier orbitals of the cluster are localised at the surface.
5. Making a complex issue one-dimensional in a referendum causes instabilities which can lead to societal displacements.
6. In a (EDO-TTF)<sub>4</sub>(PF<sub>6</sub>)<sub>2</sub> tetramer cluster, a 0110 charge ordered state is more stable compared to a situation with delocalised holes and this is predominantly due to the gain of induction energy.
7. Calculated properties of the bistable dithiazolyl molecular crystal, obtained with a frozen X-ray geometry, differ from those obtained by vibrational averaging [3]. This is not the case for the properties of (EDO-TTF)<sub>2</sub>PF<sub>6</sub>, discussed in this thesis.  
3: S. Vela, M. Deumal, M. Shiga, J.J. Novoa, J. Ribas-Arino, *Chem. Sci.* 6 (2015), 2371

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<sup>a</sup> Inspired by the allegory of the cave, Plato, *The republic*, book VII

8. Under Aristotelian scholasticism, the existence of elements other than noble gases and elements beyond Beryllium ( $\text{Be}$ ,  $1s^2 2s^2$ ) is difficult to conceive.
9. Het getuigt van wijsheid te weten waar de grens van de systeemwereld ligt en wat de bedoeling van het systeem is. Als de systeemwereld prevaleert boven de bedoeling, telt slechts de rechtlijnige uitvoering van regels.<sup>b</sup>
10. Unremunerated work is not orthogonal to professional work and a hobby is yet something different.
11. When using logic to understand a system it is often the case that a more detailed description of it is understood in terms of a more simpel model.<sup>c</sup>
12. Fans of history will be more happy in the future.<sup>d</sup>
13. I propose the possibility of human-entanglement after recent proof of quantum-entanglement.<sup>e</sup>
14. In music, it are the expectations of the listener that are played.<sup>f</sup>

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<sup>b</sup> Based on *"Verdraaide Organisaties – Terug naar de bedoeling."*, Wouter Hart, Kluwer, 2012

<sup>c</sup> Based on a question by Renske Linker in 2013: *"Wat is logisch eigenlijk?"*

<sup>d</sup> Based on a statement by Dirk Linker in 2013: *"Wanneer je in de toekomst zou leven dan is er meer geschiedenis."*

<sup>e</sup> Based on a quote used by Francien Linker in 2015: *"Distance means so little, when someone means so much."*

<sup>f</sup> Based on a statement by Arjan Linker in 2016: *"In good music, surprise and regularity are well-balanced."*